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A DENSITY FUNCTION THEORY (DFT) STUDY OF THE PROPOSED INSENSITIVE HIGH ENERGY DENSITY MATERIAL (IHEDM): 2-AZA-3-DINITROMETHYLENE-4-AZANITRO BICYCLO [3.3.0]-7-NITRO-6,8 DIAZOLE (ADAND)

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14. ABSTRACT

A theoretical analysis of the proposed insensitive high energy density material (IHEDM) 2-aza-3-dinitromethylene-4-azanitro bicyclo [3.3 .0]-7-nitro-6,8-diazole (ADAND) is reported. A Density Functional Theory (DFT) study is performed in order to determine the optimized structure and stability as well as thermochemical aspects of ADAND. All calculations were performed using the Gaussian03 software with the Gaussview graphical user interface. Normal modes of vibration and heat of detonation of the proposed insensitive energetic material are calculated; the oxygen balance and energy density of the proposed IHEDM are also determined. Calculations were also performed on FOX-7; 2,4-dinitroimidazole (2,4-DNI); RDX ; 2-methyl-4,5-dinitro-l,2,3-triazole-2-oxide (MDNTO); and HMX to enable comparison of the chosen explosive performance parameters to ADAND.

15. SUBJECT TERMS

2-aza-3-dinitromethylene-4-azanitro bicyclo [3.3 .OJ-7-nitro-6,8-diazole (ADAND); 2,4-dinitroimidazole (2,4-DNI); I,I-diamino-2,2-dinitroethene (DADNE), FOX-7; RDX; HMX; 2-methyl-4,5-dinitro-l,2,3-triazole-2-oxide (MDNTO); Density functional theory (DFT); B3LYP; Vibrational modes, Heat of detonation; Oxygen balance (OB); Energy density (molecular); and Composite volumetric energy density (CVED)

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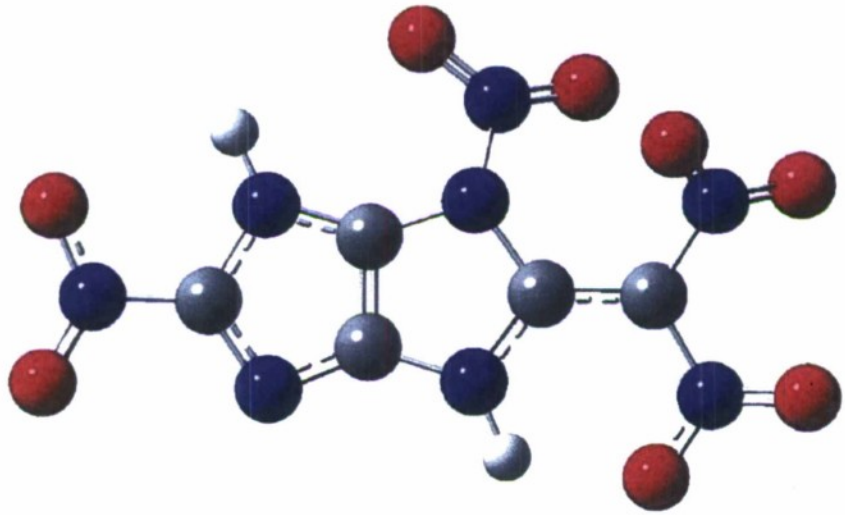
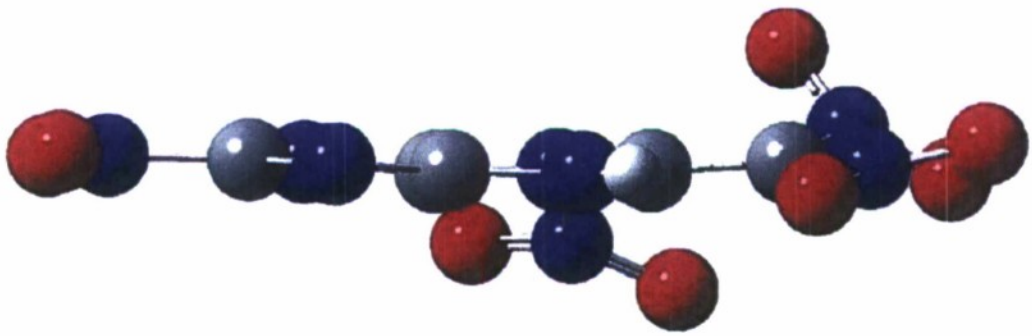
CONTENTS

SUMMARY

The stability and thermochemistry of a proposed "bicyclo-" derivative of the known insensitive high energy density materials (IHEDMs) FOX-7 (l,l-diamino-2,2-dinitroethene-DADNE) and 2,4-dinitroimidazole (2,4-DNI) is assessed using the Density Functional Theory (DFT) as implemented in Gaussian03. The optimized structure of the proposed energetic, 2-aza-3-dinitromethylene-4-azanitro bicycle [3.3.0]-7-nitro-6,8-diazole (ADAND), is illustrated in figure 1a and b. The DFT results demonstrate that ADAND is indeed stable on the molecular potential energy surface with energy density and heat of detonation characteristics superior to FOX-7, RDX, and HMX. In particular, ADAND possesses a molecular energy density 24% greater than RDX and 53% greater than 2,4-DNI, and a heat of detonation 93% greater than 2-methyl-4,5-dinitro-l,2,3-triazole-2-oxide (MDNTO), and 26% greater than HIVIX. Thermochemistry results and volumetric-energy density calculations indicate that this molecule is superior overall to HMX, FOX-7, RDX, MDNTO, and 2,4-DNI and may also possess significant potential for applications where explosive or propellant properties may be pursued and tuned in a single molecular configuration.



B3LYP/6-31g(d) optimized structure top view



B3LYP/6-31g(d) optimized structure side view

Figure 1
ADAND
(grey = carbon, blue = nitrogen; red = oxygen, white = hydrogen)

INTRODUCTION

In organic chemistry, the structures of some rings of atoms are unexpectedly stable. Aromaticity is a chemical property in which a conjugated ring of unsaturated bonds, lone pairs, or empty orbitals exhibit stabilization stronger than would be expected by the stabilization of conjugation alone. It can also be considered a manifestation of cyclic delocalization and of resonance. Moreover, the presence of hydrogen bonding in molecules also signals greater stability than what would be expected. These characteristics ultimately equate to a general trend toward decreased impact and friction sensitivity when present in energetic materials.

The ADAND is essentially a bicyclo-aza derivative of the well-known IHEDM's 2,4-DNI and FOX-7 and is expected to possess equivalent insensitivities due to availability of inter- and intra-molecular hydrogen bonds and electron delocalization with enhanced volumetric power characteristics due to the additional molar volume of decomposition products.

METHODS, ASSUMPTIONS, AND PROCEDURES

Computational details: DFT was applied in this study as implemented in Gaussian03. For the Kohn-Sham Hamiltonian, a generalized gradient approximation is included in Becke's exchange correlation functional B3LYP. This three-parameter hybrid functional was paired with a valence double-zeta polarized basis set; i.e., 6-3 lg(d). This pairing represents a reasonable level of theory and basis set complexity, which duplicates gas-phase heats of formation and heats of reaction for CNOH-containing molecules with good to excellent accuracy.

For calculation of the oxygen balance (OB), the following approach was used: for an explosive that contains some or all of the following atoms: aluminum, boron, carbon, calcium, chlorine, fluorine, hydrogen, potassium, nitrogen, sodium, and oxygen (with the formula Al_{al}, B_b, C_c, Ca_{ca}, Cl_{cl}, F_f, H_h, K_k, Na_{na}, O_o), the oxygen balance (OB%) will be

$$-\frac{32\{0.75al+0.75b+1c+0.5ca-0.25f+0.25f+0.25h+0.25k+0n+0.25na-0.05o\}}{explosive\ molecular\ weight}\ x\ 100,$$

where the indices - al, b, c, ca, cl, f, h, k, n, na, and o denote the number of atoms of each element in a mole of the explosive composition. The contribution of nitrogen to the oxygen balance is zero, since it does not bind to the other elements.

The heats of reaction (i.e., detonation - ΔH°_{det}) for the respective molecules were determined as ΔH°_f (products) - ΔN°_f (reactants) using the thermochemical output from the Gaussian DFT calculations.

The molecular energy density values were calculated from the heats of reaction results and the molecular masses: Energy Density (KJ/gram) = (KJ/mole) (moles/gram).

The explosion of one mole of ADAND produces 10 molar volumes, as can be seen from the stochiometrically balanced equation shown in the next section. These molar volumes at 0°C and atmospheric pressure form an actual volume of (10 moles)(22.4 L/mole) = 224 L. Using Charles' law, this volume can be calculated for other temperatures; for example, at 15°C (288.15K), $V_{15^\circ C}$ = (22.4 L/mole)(288.15/273.I5) = 23.64 L/mole. Therefore, at 15°C, the volume of gas produced by the explosive decomposition of one mole of ADAND is: $V_{15^\circ C}$ = (23.64 L/mole)(10 moles) = 236.4 L. As a measure of performance, the Composite Volumetric-Energy Density (CVED) = (Energy Density)(Volume of gas produced) was introduce. The CVED results are tabulated in table 2.

RESULTS AND DISCUSSION

The results of the normal mode analysis (fig. 2) for the proposed IHEDM structure yielded no imaginary frequencies for the 3N–6 vibrational degrees of freedom, where N is the number of atoms in the system. This indicates that the structure of the ADAND molecule corresponds to at least a local minimum on the potential energy surface. Figure 2 also includes the specific infrared and Raman frequencies for future reference should the synthesis and characterization of ADAND be pursued.

In order to estimate the amount of energy available for release upon detonation, the Kistiakowsky-Wilson rules need to be applied, which state that (for an explosive with an OB not below -40%):

1. Carbon atoms are converted to CO
2. Any remaining oxygen is used to convert hydrogen atoms to H_2O
3. Any oxygen remaining after no. 2 is satisfied is used to convert CO to CO_2
4. All nitrogen atoms are converted to N_2

Applying these rules to ADAND, FOX-7, RDX, and HIVIX the following ratios of detonation products are predicted:

ADAND: $C_5N_8O_8H_2 \rightarrow 3CO + 1H_2O + 2CO_2 + 4N_2$
FOX-7: $C_2N_4O_4H_4 \rightarrow 2CO + 2H_2O + 2N_2$
2,4-DNI: $C_3N_4O_4H_2 \rightarrow 3CO + 1H_2O + 2N_2$
RDX: $C_3N_6O_6H_6 \rightarrow 3CO + 3H_2O + 3N_2$
HMX: $C_4N_8O_8H_8 \rightarrow 4CO + 4H_2O + 4N_2$
MDNTO: $C_3O_5N_5H_3 \rightarrow 2CO + 3/2(H_2O) + 5/2(N_2) + ¾(CO_2) + ¼(C)$

	1	2	3
	A	A	A
Frequencies --	43.4116	50.0993	68.8076
Red. masses --	14.3166	13.5418	14.5989
Frc consts --	0.0159	0.0200	0.0407
IR Inten --	2.0007	0.6550	1.4761
Raman Activ --	0.5888	1.0998	2.3282
Depolar (P) --	0.4701	0.7387	0.6210
Depolar (U) --	0.6395	0.8497	0.7662

	4	5	6
	A	A	A
Frequencies --	75.1412	81.2987	93.0765
Red. masses --	15.5564	15.4099	14.2334
Frc consts --	0.0518	0.0600	0.0727
IR Inten --	0.6635	1.1968	1.9353
Raman Activ --	1.4799	1.9302	1.0985
Depolar (P) --	0.6700	0.6823	0.5631
Depolar (U) --	0.8024	0.8112	0.7205

	7	8	9
	A	A	A
Frequencies --	112.5171	129.7963	151.7156
Red. masses --	14.1425	10.2415	13.0095
Frc consts --	0.1055	0.1017	0.1764
IR Inten --	1.7432	3.5778	0.9644
Raman Activ --	4.4898	1.2385	0.9905
Depolar (P) --	0.4181	0.2029	0.6973
Depolar (U) --	0.5897	0.3373	0.8217

Figure 2
Vibrational frequencies (normal modes) of ADAND

	10	11	12
	A	A	A
Frequencies --	190.2554	207.1817	224.1383
Red. masses --	13.8186	12.6169	13.9912
Frc consts --	0.2947	0.3191	0.4141
IR Inten --	2.4132	2.8567	5.4176
Raman Activ --	2.5183	1.2658	2.4147
Depolar (P) --	0.3692	0.7486	0.6595
Depolar (U) --	0.5393	0.8562	0.7948

	13	14	15
	A	A	A
Frequencies --	238.5793	278.0211	288.4893
Red. masses --	12.9665	13.3798	13.1894
Frc consts --	0.4348	0.6093	0.6467
IR Inten --	0.4005	4.1542	0.6194
Raman Activ --	2.4949	9.3699	17.1030
Depolar (P) --	0.6261	0.3282	0.1457
Depolar (U) --	0.7701	0.4942	0.2544

	16	17	18
	A	A	A
Frequencies --	316.3828	343.3955	402.8314
Red. masses --	15.0021	10.6088	13.2130
Frc consts --	0.8848	0.7371	1.2633
IR Inten --	1.1250	1.0858	10.0912
Raman Activ --	1.7073	2.2918	12.7799
Depolar (P) --	0.1125	0.1562	0.3962
Depolar (U) --	0.2022	0.2702	0.5676

	19	20	21
	A	A	A
Frequencies --	420.7782	431.0216	474.3897
Red. masses --	11.8853	14.6426	10.1653
Frc consts --	1.2398	1.6028	1.3478
IR Inten --	24.3829	2.9899	6.4332
Raman Activ --	5.5681	8.5741	4.8852
Depolar (P) --	0.2134	0.3374	0.6009
Depolar (U) --	0.3517	0.5045	0.7507

	22	23	24
	A	A	A
Frequencies --	489.4222	558.6336	592.9152
Red. masses --	10.8995	8.4633	3.7715
Frc consts --	1.5382	1.5561	0.7812
IR Inten --	4.2582	11.0967	54.0818
Raman Activ --	16.9902	0.5673	2.9622
Depolar (P) --	0.4170	0.4890	0.4491
Depolar (U) --	0.5886	0.6568	0.6198

	25	26	27
	A	A	A
Frequencies --	620.8797	649.2942	653.3773
Red. masses --	1.2433	7.5125	1.3457
Frc consts --	0.2824	1.8660	0.3385
IR Inten --	53.2535	4.2728	93.4048
Raman Activ --	1.3157	7.9107	0.3844
Depolar (P) --	0.5994	0.4531	0.6843
Depolar (U) --	0.7495	0.6236	0.8126

Figure 2
(continued)

	28	29	30
	A	A	A
Frequencies --	680.3458	707.5935	721.3138
Red. masses --	8.4472	13.7458	7.7250
Frc consts --	2.3037	4.0550	2.3681
IR Inten --	14.8680	8.4421	1.3080
Raman Activ --	0.7849	4.7646	5.7380
Depolar (P) --	0.4039	0.3208	0.5050
Depolar (U) --	0.5754	0.4858	0.6711

	31	32	33
	A	A	A
Frequencies --	729.9483	742.1343	752.1826
Red. masses --	12.2446	8.6069	13.1773
Frc consts --	3.8440	2.7929	4.3926
IR Inten --	27.9397	2.1547	13.4872
Raman Activ --	1.6963	2.5190	5.3609
Depolar (P) --	0.7470	0.7500	0.5062
Depolar (U) --	0.8552	0.8571	0.6721

	34	35	36
	A	A	A
Frequencies --	779.8693	795.2999	818.8794
Red. masses --	10.6927	13.5389	10.3562
Frc consts --	3.8316	5.0454	4.0916
IR Inten --	26.3990	41.0678	53.2830
Raman Activ --	24.8638	4.5643	23.0538
Depolar (P) --	0.3273	0.6401	0.1360
Depolar (U) --	0.4931	0.7806	0.2395

	37	38	39
	A	A	A
Frequencies --	821.9033	859.0781	912.9362
Red. masses --	10.8798	9.2155	9.0904
Frc consts --	4.3302	4.0072	4.4639
IR Inten --	53.9138	87.3435	43.6572
Raman Activ --	3.8247	5.6195	125.7859
Depolar (P) --	0.4679	0.4289	0.2467
Depolar (U) --	0.6375	0.6003	0.3958

	40	41	42
	A	A	A
Frequencies --	994.4403	1017.9286	1082.5008
Red. masses --	8.6087	7.9102	2.7006
Frc consts --	5.0158	4.8291	1.8645
IR Inten --	133.1869	46.9564	212.9864
Raman Activ --	152.5137	4.7128	34.7196
Depolar (P) --	0.2067	0.2985	0.7135
Depolar (U) --	0.3426	0.4598	0.8328

Figure 2
(continued)

	43	44	45
	A	A	A
Frequencies --	1115.0370	1163.2035	1207.5869
Red. masses --	6.0318	2.2804	4.9419
Frc consts --	4.4185	1.8179	4.2460
IR Inten --	7.9488	39.4075	45.1799
Raman Activ --	20.6921	3.7022	56.5432
Depolar (P) --	0.5019	0.7373	0.2557
Depolar (U) --	0.6683	0.8488	0.4073

	46	47	48
	A	A	A
Frequencies --	1263.9145	1298.4819	1337.8483
Red. masses --	5.6968	12.6006	5.4962
Frc consts --	5.3619	12.5173	5.7960
IR Inten --	33.5465	302.1242	763.8799
Raman Activ --	82.6265	348.7459	346.0043
Depolar (P) --	0.4089	0.4027	0.5102
Depolar (U) --	0.5804	0.5742	0.6757

	49	50	51
	A	A	A
Frequencies --	1363.4299	1367.8912	1387.9831
Red. masses --	13.3263	12.2590	5.8489
Frc consts --	14.5957	13.5148	6.6388
IR Inten --	880.9572	59.7193	24.4175
Raman Activ --	588.6832	73.6245	85.3694
Depolar (P) --	0.4322	0.7160	0.1622
Depolar (U) --	0.6035	0.8345	0.2791

	52	53	54
	A	A	A
Frequencies --	1403.3036	1464.8809	1542.5950
Red. masses --	4.9725	11.4831	11.4986
Frc consts --	5.7694	14.5183	16.1213
IR Inten --	28.4631	91.3583	188.5051
Raman Activ --	877.7864	72.8563	667.2161
Depolar (P) --	0.2690	0.3077	0.2580
Depolar (U) --	0.4240	0.4706	0.4101

	55	56	57
	A	A	A
Frequencies --	1590.3018	1603.0612	1624.7603
Red. masses --	9.2495	11.4979	8.8971
Frc consts --	13.7824	17.4088	13.8382
IR Inten --	4.6434	61.2750	32.5723
Raman Activ --	306.1736	73.4657	40.9754
Depolar (P) --	0.2939	0.2496	0.4114
Depolar (U) --	0.4543	0.3995	0.5830

	58	59	60
	A	A	A
Frequencies --	1634.0959	1652.1375	1670.4485
Red. masses --	8.2306	14.0970	13.7980
Frc consts --	12.9490	22.6710	22.6847
IR Inten --	254.5549	194.4901	670.6027
Raman Activ --	276.2332	26.0598	1.6461
Depolar (P) --	0.4145	0.5679	0.7184
Depolar (U) --	0.5860	0.7244	0.8361

Figure 2
(continued)

	61	62	63
	A	A	A
Frequencies --	1760.2533	3517.8813	3633.5893
Red. masses --	13.9574	1.0808	1.0824
Frc consts --	25.4803	7.8802	8.4198
IR Inten --	321.9431	156.9491	162.6587
Raman Activ --	0.5185	161.3733	54.8973
Depolar (P) --	0.7413	0.1727	0.1840
Depolar (U) --	0.8514	0.2945	0.3108

Figure 2
(continued)

From this information and the DFT calculated heats of formation of the reactants and products, the heat of reaction (i.e., detonation) can be determined as follows:

$$\Delta H^\circ_{det}\,(\text{ADAND}) = [3\Delta H^\circ_f(CO) + 1\Delta H^\circ_f(H_2O) + 2\Delta H^\circ_f(CO_2) + 4\Delta H^\circ_f(N_2)] - [-\Delta H^\circ_f\,(\text{ADAND})]$$

$$\Delta H^\circ_{det}(\text{FOX-7}) = 2\Delta H^\circ_f(CO) + 2\Delta H^\circ_f(H_2O) + 2\Delta H^\circ_f(N_2) - [-\Delta H^\circ_f\,(\text{FOX-7})]$$

$$\Delta H^\circ_{det}(\text{2,4-DNI}) = 3\Delta H^\circ_f(CO) + 1\Delta H^\circ_f(H_2O) + 2\Delta H^\circ_f(N_2) - [-\Delta H^\circ_f\,(\text{2,4-DNI})]$$

$$\Delta H^\circ_{det}(\text{RDX}) = 3\Delta H^\circ_f(CO) + 3\Delta H^\circ_f(H_2O) + 3\Delta H^\circ_f(N_2) - [-\Delta H^\circ_f\,(\text{RDX})]$$

$$\Delta H^\circ_{det}(\text{HMX}) = 4\Delta H^\circ_f(CO) + 4\Delta H^\circ_f(H_2O) + 4\Delta H^\circ_f(N_2) - [-\Delta H^\circ_f\,(\text{HMX})]$$

$$\Delta H^\circ_{det}(\text{MDNTO}) = 2\Delta H^\circ_f(CO) + 3/2\Delta H^\circ_f(H_2O) + 5/2\Delta H^\circ_f(N_2) + 3/4\Delta H^\circ_f(CO_2) + \tfrac{1}{4}(C) - [-\Delta H^\circ_f\,(\text{MDNTO})]$$

The heats of detonation for these molecules, as well as their products, are reported as the "sum of electronic and thermal energies" in atomic units (i.e., Hartrees), via the thermochemistry output calculated at the B3LYP/6-31g(d) level of theory (tables 1 and 2).

Table 1
Thermochemistry output for detonation products

	MW	ΔH°_f(au)*
CO_2	44	-188.567
CO	28	-113.302
H_2O	18	-76.385
N_2	28	-109.516
C	12	-37.844

*Sum of electronic and thermal energies as reported from the Gaussian03 DFT thermochemistry results.

Table 2
ADAND, FOX-7, RDX, HMX, MDNTO, and 2,4-DNI thermochemistry output and theoretical performance parameters

	ΔH°_{f} (au)*	MW	OB (%)	ΔH°_{det} (au/KJ/mole)	Energy density (KJ/g)	Volume (L)	CVED (KJ-L/g)
ADAND	-1230.891	302	-21.2	-0.598/-1,571	5.2	236.4	1229
FOX-7	-598.208	148	-21.6	-0.198/-519	3.5	141.84	496
2,4-DNI	-635.118	158	-30.4	-0.205/-538	3.4	141.84	482
RDX	-897.253	222	-21.6	-0.356/-935	4.2	212.76	894
HMX	-1196.336	296	-21.6	-0.476/-1250	4.2	283.68	1191
MDNTO	-765.549	189	-1.3	-0.310/-814	4.3	159.57	686

*Sum of electronic and thermal energies as reported from the Gaussian03 DFT thermochemistry results.

Note: Volume of gases calculated at 15°C.

Note that these calculations are based on rather idealized gas-phase enthalpies, and in reality, other factors such as phase transition from solid state to gaseous state, crystal and crystal packing density will be important. The point is that the ΔH°_{det} calculations are not necessarily to be taken in the absolute sense, but considered as a relative trend. In this way, more meaningful conclusions can be obtained.

CONCLUSIONS

The Density Functional Theory results of this study indicate that the newly proposed high energy density material, 2-aza-3, dinitromethylene-4-azanitro bicycle [3.3.0]-7-nitro-6,8-diazole (ADAND), has a molecular energy density nearly 50% greater than FOX-7 and 24% greater than either RDX or HMX. Further, the composite volumetric energy density of ADAND is approximately 150% greater than FOX-7, 155% greater than 2,4-DNI, and 37% greater than RDX. The optimized structure is stable on the molecular potential energy surface, as evidenced by the absence of any imaginary frequencies. Also, the optimized geometry exhibits a relatively flat molecular configuration, which would be expected to pack efficiently in its solid state crystal lattice.

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